Spin polarization and effective mass: a numerical study in disordered two dimensional systems

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We numerically study the magnetization of small metallic clusters. The magnetic susceptibility is enhanced for lower electronic densities due to the stronger influence of electron-electron interactions. The magnetic susceptibility enhancement stems mainly from an enhancement of the mass for commensurate fillings, while for non-commensurate fillings its a result of an enhancement of the Landé g factor. The relevance to recent experimental measurements is discussed.

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Much attention has recently been given to the study of interacting electrons in two-dimensional disordered systems, motivated by new experimental observations[1]. The conductance of dilute 2D electron systems show fascinating temperature and magnetic field dependencies. One of the most intriguing behaviors is the strong decrease in the critical magnetic field, B_c, needed in order to fully spin polarize the system at low densities. These low densities are characterized by a high ratio of the intra electron interaction energy E_c and the Fermi energy E_F. This ratio is denoted by $r_s = E_c/E_F$. In the weakly interacting regime ($r_s \ll 1$) the system behaves as independent non-interacting electrons with a magnetic susceptibility equal to the Pauli susceptibility $\chi = g\mu_B^2\nu$ (where g is the Landé factor, μ_B is the Bohr magneton and ν is the density of states at the Fermi energy). As the electron density is lowered, measurements show an enhancement in the susceptibility[2,3,4,5,6,7]. Although there is an ongoing debate whether these measurements support the scenario of spontaneous spin polarization[8], or just an enhanced magnetic susceptibility[6,7], it is nevertheless generally accepted that a large enhancement of the magnetic susceptibility occurs over a large region of densities corresponding to $r_s > 6$.

An interesting question raised recently[6,8] is whether to attribute the enhancement of susceptibility to an increase of the g factor or to an increase of the effective mass (the density of states in a 2D system is proportional to the effective mass). By a novel experimental method Pudalov et. al.[6] were able to measure separately χ and m as function of r_s. Although there are two different methods to extract m which do not exactly agree, nevertheless, it is clear that m increases much quicker as functions of r_s than g. Recent measurements by Shashkin et. al.[8] strengthen the case for a strong dependence of m on r_s while g turns out to be constant. This result is in contrast to theoretical considerations based on the Fermi liquid picture which predict a strong enhancement in g[9,10,11], but has some similarities to Wigner crystallization scenarios[12,13].

Since the development of a theoretical description of interacting electrons in disorder systems turns out to be rather intricate, a lot of effort has been invested in numerical studies. For example, the influence of electron-electron interactions on the persistent current and conductance has been extensively studied for small metallic clusters[14,15,16,17,18,19,20,21]. In this paper we will use exact digonalization of small clusters in order to investigate the influence of r_s on χ, g and m of disordered systems. The magnetic susceptibility is strongly enhanced as electron-electron interaction increases. Nevertheless, the susceptibility shows no clear signs of divergence at any finite value of r_s. While for commensurate fillings the enhancement in χ is mainly driven by an enhancement in the mass m, for non-commensurate systems the g factor is strongly enhanced by interactions.

The disordered interacting cluster is represented by the following tight-binding Hamiltonian:

$$\hat{H} = \sum_{k,j;\sigma} \epsilon_{k,j} n_{k,j;\sigma} - V \sum_{k,j;\sigma} [a^\dagger_{k,j+1;\sigma} a_{k,j;\sigma} + a^\dagger_{k+1,j;\sigma} a_{k,j;\sigma} + h.c.] + U_{\rm H} \sum_{k,j} n_{k,j;+\frac{1}{2}} n_{k,j;-\frac{1}{2}} + U \sum_{k,j>l,p;\sigma,\sigma'} (n_{k,j;\sigma} - K)(n_{l,p,\sigma'} - K) s/|\vec{r}_{k,j} - \vec{r}_{l,p}|, \quad (1)$$

where $\vec{r} = (k, j)$ denotes a lattice site, $a^\dagger_{k,j;\sigma}$ is an electron creation operator (with spin $\sigma = -\frac{1}{2}, +\frac{1}{2}$), the number operator is $n_{k,j;\sigma} = a^\dagger_{k,j;\sigma} a_{k,j;\sigma}$, $\epsilon_{k,j}$ is the site energy, chosen randomly between $-W/2$ and $W/2$ with uniform probability, $V = 1$ is a constant hopping matrix element, $K = n$ is a positive background charge equal to the electronic density $n = N/M$ (where N is the number of electrons and M the number of sites) and s is the lattice constant. The electron-electron interaction is composed of the on-site Hubbard interaction $U_{\rm H}$ between electrons of opposite spin and the and the long range part U. The value of U is related to the electronic density and via $U = V\sqrt{4\pi n} r_s$ and we chose $U_{\rm H} = U$[21]. Thus, the physical content of the density variation performed in experiment is captured by controlling the ratio of the Fermi energy to the interaction energy achieved simply by changing the interaction strengths U.

We consider systems composed of $N = 4$ and $N = 6$ electrons residing on 4×3, 4×5 and 6×6 lattices. We

set $W = 8$ for the smaller lattices and $W = 5$ for the larger one, so that the single particle properties correspond to a diffusive system., For each value of the interaction strength between $0 < r_s < 30$ the six lowest eigenvalues of the sectors with $S_z = 0$ and $S_z = 1$ are calculated[22] for a hundred different realizations.

Using the excitation energies it is possible to estimate the magnetic susceptibility χ and the density of states at the Fermi energy ν. Since we are dealing with a cluster of finite size for which the levels are discrete, it is reasonable to use a discrete definition of the susceptibility

$$\frac{1}{\chi^*} = \frac{\Delta B}{\Delta M} = \frac{E_1(S_z = 1) - E_1(S_z = 0)}{g\mu_B^2} = \frac{1}{g^*\mu_B^2\nu^*}, \quad (2)$$

where $E_1(S_z)$ is the lowest eigenvalue in the corresponding S_z sector. This is based on the fact that the first change in the magnetic moment of the system will occur when the applied magnetic field will be strong enough to favor the $S_z = 1$ state as a ground state. That will occur once $g\mu_B B = E_1(S_z = 1) - E_1(S_z = 0)$, resulting in $M = \mu_B$. A plot of $\langle\chi\rangle/\langle\chi^*\rangle = \langle E_1(U, S_z = 1) - E_1(U, S_z = 0)\rangle/\langle E_1(U = 0, S_z = 1) - E_1(U = 0, S_z = 0)\rangle$ (where $\langle\ldots\rangle$ denotes an average over different realizations of disorder) is presented in Fig. 1. It can be seen that χ^* is strongly enhanced as function of interaction. For small values of r_s the numerical results follow the well known Fermi liquid predictions $\chi/\chi^* = 1 - (\sqrt{2}/\pi)r_s$[23]. For higher values of r_s, a linear relation $1/\chi^* \propto 1/r_s^2 - 1/r_0^2$ (see Fig. 2) between the inverse magnetic susceptibility and $1/r_s^2$ is observed. From this relation one might extrapolate $1/\chi^* = 0$ at $r_s = r_0$, i.e., full spin polarization at finite density. Noting that $1/r_s^2$ corresponds to the electronic density n and that $1/\chi^*$ is proportional to the magnetic field B_c needed to fully polarize the system, this relation may be rewritten as $B_c \propto n - n_0$ which is exactly an empirical relation proposed in Ref.[8] based on experimental observations. Nevertheless, at large values of r_s the growth in χ^* seems to tapper off, resulting in no clear evidence of divergence in χ^* for the diffusive regime, although partial spin polarization is seen for part of these realizations[22].

As in the experimental measurements, the main problem in interpreting the enhancement in χ^* is that it might originate from and enhancement in the g^* (i.e., the result of some exchange mechanism) or it might result from a change in the density of states ν^* which is unrelated to the spin. Nevertheless, it is possible to differentiate both effects using the following consideration. When a strong enough magnetic field is applied on a system, the system will switch from the zero magnetic field ground state to the first excited state with higher spin. This process is depicted in Eq. (2) and involves both the density of states and exchange. In the Landau quasi-particle description[24] $\chi^*/\chi = m^*g^*/mg$, where $g/g^* = (1 + F_0^a)$ and $m^*/m = 1 + F_1^s/2$, and $F^{s(a)}$ are the usual singlet (triplet) Fermi liquid parameters. Thus, both the singlet and triplet Fermi liquid parameters play a role. On the other hand, when one excites the system from the lowest singlet state to the first excited singlet state, only the density of states (i.e., m, or the singlet Fermi liquid parameter) plays a role. The latter is accessible via the level spacing between the two lowest excitations of the $S_z = 0$ sector with total spin zero. They can be easily identified since states in the $S_z = 0$ sector which have a total spin larger than zero, have the same energy as their counterpart in the $S_z = 1$ sector (with no magnetic field the energy of an $S = 1, S_z = 0$ state is equal to the energy of a $S = 1, S_z = 1$ state). Thus we identify the two lowest states in the $S_z = 0$ which are not degenerate

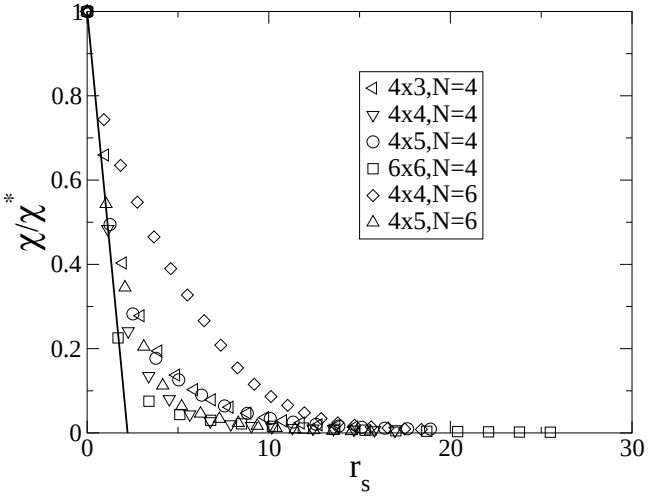

FIG. 1: The inverse magnetic susceptibility χ/χ^* as function of r_s for different lattice sizes and number of electrons. The line corresponds to $1 - (\sqrt{2}/\pi)r_s$ which is the Fermi liquid correction to the susceptibility. As the interaction increases the susceptibility deviates from the Fermi liquid description

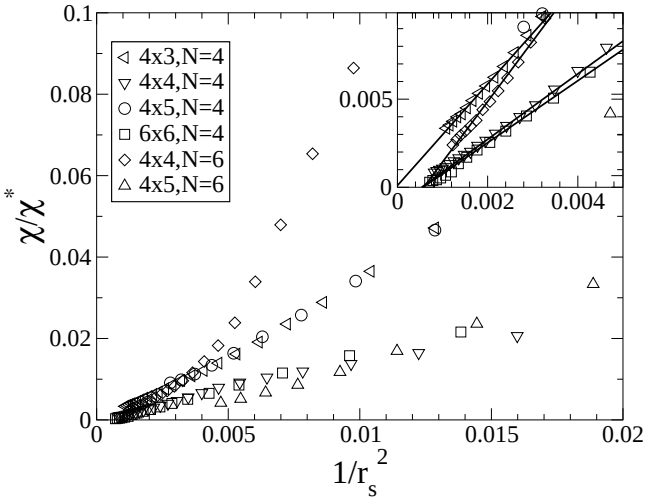

FIG. 2: The inverse magnetic susceptibility χ/χ^* as function of $1/r_s^2$ (which corresponds to the electronic density n) for strong interactions. The inset focuses on the region of strong interactions. The lines correspond to a linear fit of the form $1/\chi^* \propto 1/r_s^2 - 1/r_0^2$.

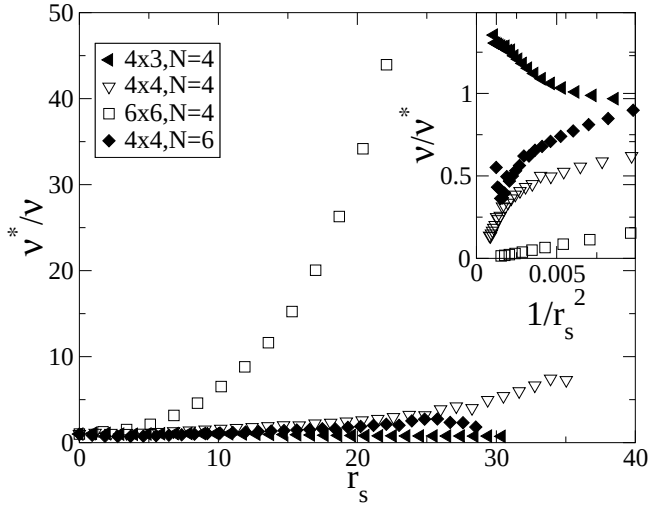

FIG. 3: The single electron density of states ν^* for different lattice sizes and number of electrons. filled symbols correspond to non-commensurate fillings, while empty symbols to commensurate ones. Inset: behavior of ν^* at strong interactions. The density of states (i.e.,the mass) strongly increases for the commensurate fillings, while it shows no signs of divergence for non-commensurate fillings.

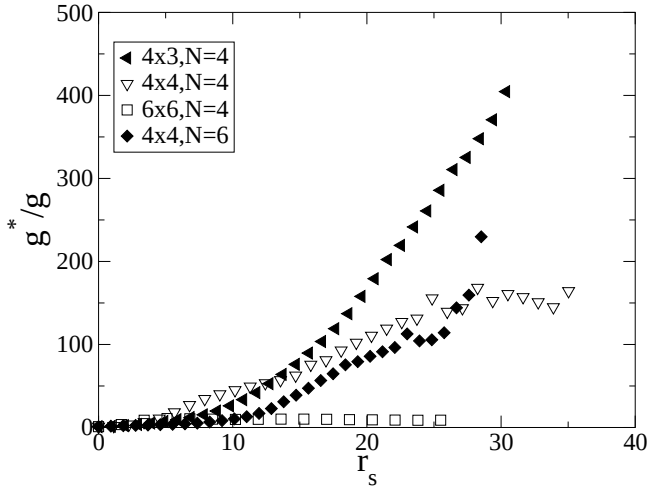

FIG. 4: The Landé g factor g^* for different lattice sizes and number of electrons. The g factor is strongly enhanced for the non-commensurate fillings, while it saturates for the commensurate ones.

with states in the $S_z = 1$ sector: $E_1(S = 0), E_2(S = 0)$ leading to

$$\nu^* = \frac{1}{\langle E_2(S=0) - E_1(S=0)\rangle}. \qquad (3)$$

A plot of ν^*/ν is shown in Fig. 3, while $g^*/g = \nu^*\chi/\nu\chi^*$ is presented in Fig. 4. A very different behavior between the density of states and the g factor is seen. There is a strong enhancement of the density of state as function of the interaction strength for commensurate fillings, while the g factor is strongly enhanced for the non-commensurate fillings. Thus, for fillings which are prone to Wigner crystallization (commensurate fillings) the mass is enhanced , while for frustrated systems (non-commensurate systems) the g factor is enhanced. Although both the 4×4 and 6×6 lattices are at a commensurate filling for $N = 4$ it is interesting to note that the 6×6 system shows a strong enhancement in the effective mass beginning at $r_s \sim 5$, while the 4×4 show a strong enhancement of m only much latter ($r_s \sim 30$) which is in the vicinity of the expected Wigner crystallization transition[25]. We shall comment on this later.

Although it is rather doubtful to claim that these results on small clusters are directly applicable for the experiment performed on macroscopic samples, it is interesting nevertheless to note that the behavior depicted here is in line with the recent experimental observations[6,7,8]. For not to low electronic densities all groups agree that the critical magnetic field needed to completely polarize the electronic spin is proportional to $(n - n_0)$, which is similar to the behavior seen in this study. Once lower densities are considered there is a disagreement between the experimentalist. In Ref.[8] it is claimed that the linear relation holds even for low densities and is a reliable method to find the critical density for which full polarization occurs. On the other hand, in Ref.[7] doubts are raised on the applicability of the linear relation to low densities, and whether a critical density exist. Our numerical studies of small cluster seem to be more in line with the latter, since we see deviations from the linear dependence at low densities and do not see a clear indication of full polarization at any finite density. Nevertheless, our clusters are to small to draw firm conclusions on this point.

Another interesting point is the different behavior of the mass and g factor as function of r_s between the commensurate and non-commensurate fillings. If exchange interactions lead the to the enhancement of the susceptibility, the g factor should be strongly enhanced, while if Wigner crystallization is responsible for the susceptibility behavior the mass should increase. Indeed, the dilute commensurate system (6×6, $N = 4$), which turns into a Wigner crystal at large r_s, shows a strong enhancement in the mass much prior to the expected Wigner crystallization. The non-commensurate fillings (4×3, $N = 4$ and 4×4, $N = 6$), which do not show Wigner crystallization at large r_s due to frustration, show an enhancement in g^* but not in ν^*. The commensurate system (4×4, $N = 4$) shows a rather mixed behavior, where both g^* and ν^* are enhanced. We believe this is due to the high filling which leads to a strong influence of exchange correlations. Nevertheless, once r_s is large enough, g^* saturates, while ν continues to grow. In the experimental systems, which are believed to exhibit Wigner crystallization, the large enhancement in the magnetic susceptibility is attributed[6,8] to the enhancement of the mass. The samples used in those experiments are in the dilute limit and there is no reason for frustration, i.e., they are best described by the dilute commensurate system (6×6,

$N = 4$). Thus, the numerical results seem to reproduce some of the experimental behavior rather well.

In conclusion, we have numerically studied the magnetization of small metallic clusters. The magnetic susceptibility is enhanced by electron-electron interactions, i.e., lower electronic densities. This enhancement stems mainly from an enhancement of the mass in the commensurate filling. This has some similarities to the experimental behavior recently measured.

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